Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 11:09 PM EDT

PDB ID	:	6BUR
Title	:	Crystal structures of cyanuric acid hydrolase from Moorella thermoacetica complexed with barbituric acid
Authors	:	Shi, K.; Aihara, H.
Deposited on	:	2017-12-11
Resolution	:	2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

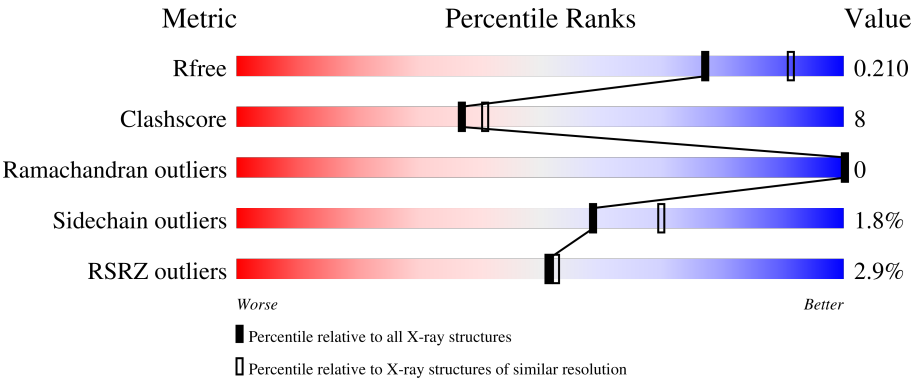
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	90% 10%
1	B	363	89% 10%
1	C	363	88% 11%
1	D	363	10% 73% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR8	A	401[A]	-	X	-	-
2	BR8	B	401	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11266 atoms, of which 18 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyanuric acid amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2697	1668	481	533	15			
1	B	363	Total	C	N	O	S	0	5	0
			2736	1692	490	539	15			
1	C	362	Total	C	N	O	S	0	0	0
			2681	1659	479	529	14			
1	D	362	Total	C	N	O	S	0	0	0
			2681	1659	479	529	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q2RGM7
A	103	ALA	GLN	engineered mutation	UNP Q2RGM7
A	104	ALA	GLU	engineered mutation	UNP Q2RGM7
A	107	ALA	LYS	engineered mutation	UNP Q2RGM7
A	279	ILE	LEU	engineered mutation	UNP Q2RGM7
A	280	ARG	LYS	engineered mutation	UNP Q2RGM7
A	281	SER	PHE	engineered mutation	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	ALA	deletion	UNP Q2RGM7
A	283	ASP	GLU	engineered mutation	UNP Q2RGM7
A	290	MET	LEU	engineered mutation	UNP Q2RGM7
A	291	ASP	ALA	engineered mutation	UNP Q2RGM7
A	292	ARG	LYS	engineered mutation	UNP Q2RGM7
B	0	HIS	-	expression tag	UNP Q2RGM7
B	103	ALA	GLN	engineered mutation	UNP Q2RGM7
B	104	ALA	GLU	engineered mutation	UNP Q2RGM7
B	107	ALA	LYS	engineered mutation	UNP Q2RGM7
B	279	ILE	LEU	engineered mutation	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ARG	LYS	engineered mutation	UNP Q2RGM7
B	281	SER	PHE	engineered mutation	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	ALA	deletion	UNP Q2RGM7
B	283	ASP	GLU	engineered mutation	UNP Q2RGM7
B	290	MET	LEU	engineered mutation	UNP Q2RGM7
B	291	ASP	ALA	engineered mutation	UNP Q2RGM7
B	292	ARG	LYS	engineered mutation	UNP Q2RGM7
C	0	HIS	-	expression tag	UNP Q2RGM7
C	103	ALA	GLN	engineered mutation	UNP Q2RGM7
C	104	ALA	GLU	engineered mutation	UNP Q2RGM7
C	107	ALA	LYS	engineered mutation	UNP Q2RGM7
C	279	ILE	LEU	engineered mutation	UNP Q2RGM7
C	280	ARG	LYS	engineered mutation	UNP Q2RGM7
C	281	SER	PHE	engineered mutation	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	ALA	deletion	UNP Q2RGM7
C	283	ASP	GLU	engineered mutation	UNP Q2RGM7
C	290	MET	LEU	engineered mutation	UNP Q2RGM7
C	291	ASP	ALA	engineered mutation	UNP Q2RGM7
C	292	ARG	LYS	engineered mutation	UNP Q2RGM7
D	0	HIS	-	expression tag	UNP Q2RGM7
D	103	ALA	GLN	engineered mutation	UNP Q2RGM7
D	104	ALA	GLU	engineered mutation	UNP Q2RGM7
D	107	ALA	LYS	engineered mutation	UNP Q2RGM7
D	279	ILE	LEU	engineered mutation	UNP Q2RGM7
D	280	ARG	LYS	engineered mutation	UNP Q2RGM7
D	281	SER	PHE	engineered mutation	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	ALA	deletion	UNP Q2RGM7
D	283	ASP	GLU	engineered mutation	UNP Q2RGM7
D	290	MET	LEU	engineered mutation	UNP Q2RGM7
D	291	ASP	ALA	engineered mutation	UNP Q2RGM7

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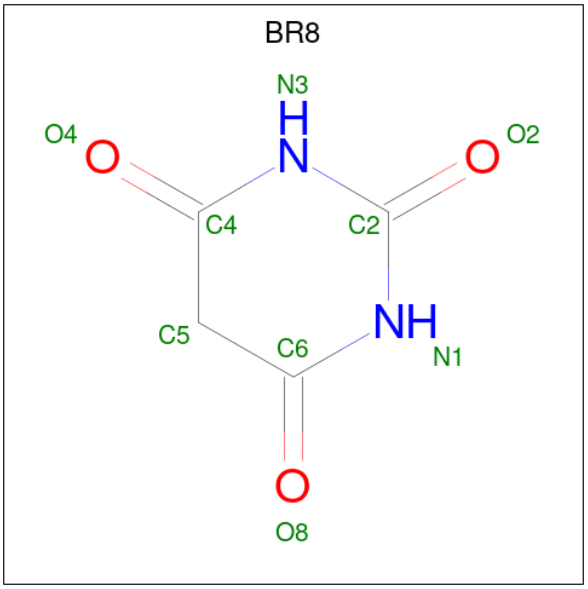
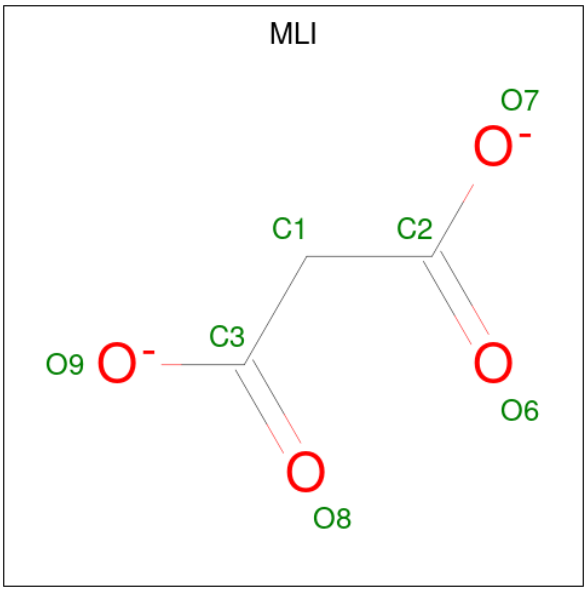
Chain	Residue	Modelled	Actual	Comment	Reference
D	292	ARG	LYS	engineered mutation	UNP Q2RGM7

- Molecule 2 is BARBITURIC ACID (three-letter code: BR8) (formula: $C_4H_4N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	1
			13	4	4	2	3		
2	B	1	Total	C	H	N	O	0	0
			13	4	4	2	3		
2	C	1	Total	C	H	N	O	0	0
			13	4	4	2	3		
2	D	1	Total	C	H	N	O	0	0
			13	4	4	2	3		

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 9 3 2 4	0	1

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

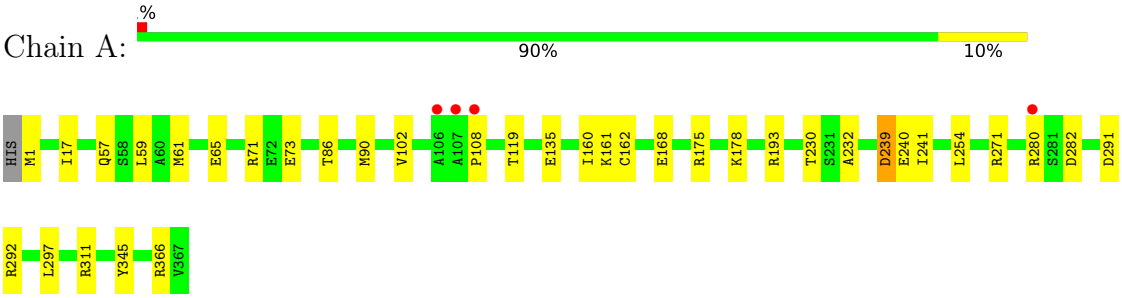
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	B	116	Total O 116 116	0	0
5	C	108	Total O 108 108	0	0
5	D	51	Total O 51 51	0	0

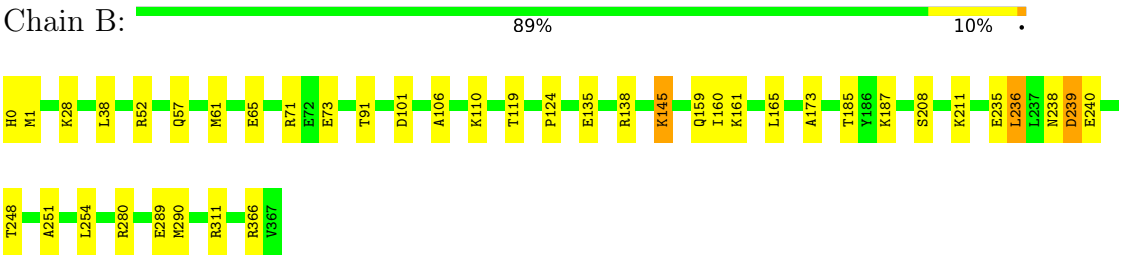
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

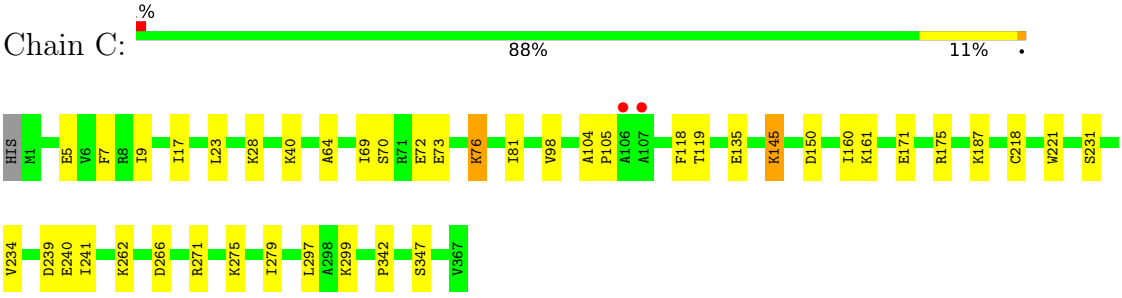
• Molecule 1: Cyanuric acid amidohydrolase



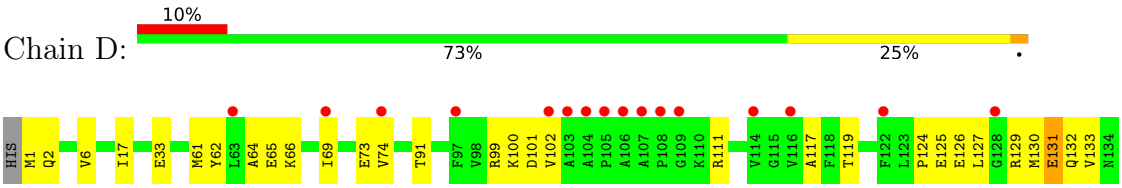
• Molecule 1: Cyanuric acid amidohydrolase

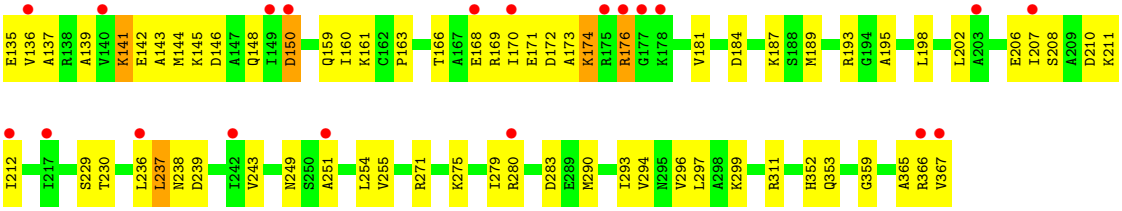


• Molecule 1: Cyanuric acid amidohydrolase



• Molecule 1: Cyanuric acid amidohydrolase




E135
V136
A137
R138
A139
V140
K141
E142
A143
M144
K145
D146
A147
Q148
I149
D150
Q159
I160
K161
C162
P163
T166
A167
E168
R169
I170
E171
D172
A173
K174
R175
R176
G177
K178
V181
D184
K187
S188
M189
R193
G194
A195
L198
L202
A203
E206
I207
S208
A209
D210
K211
I212
I217
S229
T230
L236
L237
N238
D239
I242
V243
N249
S250
A251
L254
V255
R271
K275
I279
R280
D283
E289
M290
I293
V294
M295
V296
L297
A298
K299
R311
H352
Q353
G359
A365
R366
V367

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.08Å 89.12Å 199.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.18 81.35 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.72-2.18) 99.1 (81.35-2.18)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2981: ???)	Depositor
R, R_{free}	0.163 , 0.212 0.165 , 0.210	Depositor DCC
R_{free} test set	3795 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, CA, BR8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/2729	0.54	0/3693
1	B	0.43	0/2769	0.56	0/3746
1	C	0.38	0/2713	0.54	0/3672
1	D	0.32	0/2713	0.49	0/3672
All	All	0.40	0/10924	0.53	0/14783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2697	0	2716	28	0
1	B	2736	0	2753	39	0
1	C	2681	0	2705	30	0
1	D	2681	0	2705	80	0
2	A	9	4	4	1	0
2	B	9	4	4	1	0
2	C	9	4	4	0	0
2	D	9	4	4	0	0
3	A	7	2	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	131	0	0	5	0
5	B	116	0	0	0	0
5	C	108	0	0	0	0
5	D	51	0	0	1	0
All	All	11248	18	10897	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:HD11	1:D:163:PRO:HG2	1.48	0.94
1:C:171:GLU:OE1	1:C:175:ARG:NH2	2.04	0.90
1:A:71:ARG:NH2	1:B:65:GLU:OE2	2.10	0.84
1:D:275:LYS:HE3	1:D:280:ARG:HA	1.59	0.83
1:D:275:LYS:HG3	1:D:280:ARG:HG3	1.61	0.81
1:D:207:ILE:HD11	1:D:212:ILE:HD11	1.62	0.80
1:D:33:GLU:OE2	1:D:100:LYS:HD3	1.81	0.79
1:C:72:GLU:O	1:C:76:LYS:HG3	1.85	0.77
1:A:57:GLN:OE1	1:B:57:GLN:NE2	2.17	0.75
1:D:271:ARG:O	1:D:275:LYS:HD3	1.88	0.73
1:D:1:MET:CE	1:D:251:ALA:HB2	2.19	0.73
1:D:17:ILE:HD12	1:D:62:TYR:CD1	2.25	0.71
1:B:1:MET:HE1	1:B:106:ALA:HA	1.72	0.71
1:D:141:LYS:O	1:D:145:LYS:HG2	1.91	0.70
1:C:161:LYS:HE2	1:C:231:SER:O	1.91	0.70
1:C:5:GLU:HB2	1:C:98:VAL:CG1	2.22	0.70
1:B:236[A]:LEU:HD13	1:B:238:ASN:O	1.92	0.69
1:D:150:ASP:N	1:D:150:ASP:OD1	2.26	0.68
1:A:168:GLU:OE2	5:A:502:HOH:O	2.12	0.68
1:A:65:GLU:OE2	1:B:71[A]:ARG:NH2	2.25	0.67
1:D:124:PRO:HG2	1:D:173:ALA:HB2	1.77	0.66
1:D:148:GLN:OE1	1:D:249:ASN:ND2	2.30	0.65
1:B:1:MET:CE	1:B:106:ALA:HA	2.27	0.65
1:D:141:LYS:O	1:D:145:LYS:HE2	1.97	0.64
1:D:171:GLU:O	1:D:176:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61[B]:MET:HG3	1:A:71:ARG:HD3	1.79	0.63
1:D:275:LYS:HD2	1:D:279:ILE:O	1.99	0.62
1:D:254:LEU:HD23	1:D:366:ARG:HA	1.81	0.62
1:D:130:MET:SD	1:D:212:ILE:HG22	2.40	0.62
1:C:271:ARG:O	1:C:275:LYS:HG2	1.99	0.61
1:A:271:ARG:NH1	5:A:501:HOH:O	2.11	0.61
1:D:100:LYS:HG3	1:D:102:VAL:HG13	1.82	0.61
1:B:236[A]:LEU:O	1:B:236[A]:LEU:HD12	2.00	0.60
1:D:139:ALA:HA	1:D:142:GLU:HG2	1.83	0.60
1:D:2:GLN:HA	1:D:101:ASP:HA	1.83	0.60
1:D:160:ILE:HB	1:D:230:THR:HG22	1.84	0.59
1:B:145:LYS:HE3	1:B:145:LYS:HA	1.85	0.59
1:C:275:LYS:HD3	1:C:279:ILE:O	2.02	0.59
1:C:5:GLU:HB2	1:C:98:VAL:HG13	1.83	0.59
1:D:166:THR:O	1:D:170:ILE:HG12	2.03	0.58
1:B:1:MET:CE	1:B:251:ALA:HB2	2.33	0.58
1:B:187:LYS:HD3	1:C:187:LYS:NZ	2.19	0.57
1:C:64:ALA:HB1	1:C:69:ILE:O	2.05	0.57
1:D:99:ARG:NH1	1:D:146:ASP:OD2	2.38	0.56
1:D:66:LYS:HA	1:D:66:LYS:HE2	1.87	0.56
1:D:189:MET:O	1:D:193:ARG:HG3	2.05	0.56
1:B:135:GLU:OE2	1:B:138:ARG:NH2	2.34	0.56
1:A:280:ARG:HB2	1:A:280:ARG:NH1	2.21	0.56
1:B:280:ARG:HG3	1:B:289:GLU:OE1	2.06	0.56
1:C:119:THR:HB	1:C:135:GLU:HG3	1.87	0.56
1:D:125:GLU:O	1:D:129:ARG:NH1	2.36	0.56
1:A:178:LYS:HE2	5:A:524:HOH:O	2.07	0.55
1:B:61[B]:MET:O	1:B:65:GLU:HG3	2.06	0.55
1:A:297:LEU:HD23	1:A:345:TYR:HB3	1.86	0.55
1:D:168:GLU:OE1	1:D:168:GLU:N	2.40	0.55
1:D:126:GLU:HG2	1:D:131:GLU:HG3	1.88	0.55
1:C:70:SER:OG	1:C:73:GLU:HG2	2.06	0.55
1:A:108:PRO:O	5:A:503:HOH:O	2.18	0.55
1:C:104:ALA:HB1	1:C:105:PRO:HD2	1.89	0.55
1:D:206:GLU:HA	1:D:206:GLU:OE1	2.08	0.54
1:A:240:GLU:C	1:A:241:ILE:HD12	2.28	0.54
1:A:61[B]:MET:CG	1:A:71:ARG:HD3	2.37	0.54
1:D:137:ALA:CB	1:D:202:LEU:HD23	2.37	0.54
1:D:207:ILE:CD1	1:D:212:ILE:HD11	2.36	0.54
1:D:208:SER:OG	1:D:211:LYS:HD3	2.07	0.54
1:B:124:PRO:HG2	1:B:173:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HE3	1:C:145:LYS:HA	1.90	0.53
1:C:297:LEU:N	1:C:297:LEU:HD12	2.23	0.53
1:D:169:ARG:HA	1:D:172:ASP:HB3	1.91	0.53
1:B:254:LEU:HD23	1:B:366:ARG:HA	1.91	0.53
1:D:161:LYS:CG	1:D:236:LEU:HD21	2.40	0.52
1:D:119:THR:HB	1:D:135:GLU:HG3	1.90	0.52
1:D:163:PRO:HD3	1:D:238:ASN:O	2.10	0.52
1:C:81:ILE:HG23	1:C:161:LYS:HB2	1.92	0.52
1:A:73:GLU:OE1	5:A:504:HOH:O	2.19	0.51
1:D:127:LEU:HD11	1:D:163:PRO:CG	2.30	0.51
1:A:292:ARG:NE	1:A:366:ARG:O	2.34	0.50
1:B:0:HIS:HA	1:B:101:ASP:OD1	2.11	0.50
1:D:61:MET:O	1:D:65:GLU:HG2	2.11	0.50
1:B:52:ARG:HD3	2:B:401:BR8:O2	2.11	0.50
1:D:17:ILE:HG12	5:D:518:HOH:O	2.10	0.50
1:B:311:ARG:HB3	1:D:91:THR:OG1	2.11	0.50
1:D:172:ASP:HA	1:D:176:ARG:CZ	2.42	0.50
1:B:160:ILE:HA	1:B:240:GLU:O	2.11	0.50
1:B:165:LEU:O	1:B:185:THR:HG23	2.11	0.50
1:B:57:GLN:O	1:B:61[A]:MET:HG3	2.12	0.50
1:B:1:MET:HE2	1:B:251:ALA:HB2	1.94	0.49
1:D:1:MET:HE3	1:D:251:ALA:HB2	1.91	0.49
1:D:117:ALA:HB1	1:D:142:GLU:OE2	2.13	0.49
1:D:299:LYS:HE2	1:D:353:GLN:OE1	2.13	0.48
1:B:61[A]:MET:O	1:B:65:GLU:HG3	2.13	0.48
1:D:198:LEU:HD21	1:D:352:HIS:ND1	2.29	0.48
1:A:291:ASP:OD1	1:A:291:ASP:N	2.47	0.48
1:C:218:CYS:HA	1:C:221:TRP:CH2	2.49	0.48
1:D:17:ILE:HD12	1:D:62:TYR:CG	2.48	0.48
1:B:145:LYS:HE3	1:B:145:LYS:CA	2.44	0.48
1:D:279:ILE:HD11	1:D:365:ALA:HB2	1.96	0.48
1:C:262:LYS:HG2	1:C:266:ASP:OD2	2.13	0.47
1:D:133:VAL:HG22	1:D:195:ALA:O	2.15	0.47
1:D:143:ALA:HB1	1:D:243:VAL:HG12	1.97	0.47
1:D:66:LYS:HE2	1:D:66:LYS:CA	2.43	0.47
1:C:234:VAL:HG22	1:C:234:VAL:O	2.14	0.47
1:D:189:MET:HB3	1:D:193:ARG:NH1	2.29	0.47
1:C:299:LYS:HD2	1:C:347:SER:HB3	1.96	0.47
1:D:64:ALA:HB1	1:D:69:ILE:O	2.15	0.47
1:D:132:GLN:O	1:D:136:VAL:HG23	2.15	0.47
1:D:161:LYS:HG3	1:D:236:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:VAL:C	1:D:297:LEU:HD12	2.34	0.47
1:B:61[A]:MET:HG2	1:B:71[A]:ARG:HD3	1.97	0.47
1:A:254:LEU:HD23	1:A:366:ARG:HA	1.97	0.46
1:B:235[B]:GLU:HA	1:B:235[B]:GLU:OE1	2.13	0.46
1:D:6:VAL:HB	1:D:294:VAL:HG11	1.98	0.46
1:A:17:ILE:HG22	1:A:59:LEU:HD23	1.98	0.46
1:D:66:LYS:HA	1:D:66:LYS:CE	2.45	0.46
1:D:69:ILE:HD11	1:D:74:VAL:HG22	1.97	0.46
1:D:17:ILE:HD12	1:D:62:TYR:HB2	1.98	0.46
1:D:255:VAL:HG13	1:D:367:VAL:HG12	1.97	0.46
1:A:241:ILE:HD12	1:A:241:ILE:N	2.31	0.46
1:B:208:SER:OG	1:B:211:LYS:HG2	2.16	0.45
1:C:17:ILE:C	1:C:17:ILE:HD12	2.37	0.45
1:A:193:ARG:HD3	2:A:401[A]:BR8:O8	2.17	0.45
1:C:160:ILE:HG12	1:C:241:ILE:HG13	1.97	0.45
1:D:126:GLU:CG	1:D:131:GLU:HG3	2.47	0.45
1:B:161:LYS:O	1:B:239:ASP:HA	2.17	0.45
1:D:275:LYS:CE	1:D:280:ARG:HA	2.40	0.45
1:A:162:CYS:O	1:A:232:ALA:HA	2.17	0.45
1:D:100:LYS:HE3	1:D:102:VAL:HG12	1.98	0.45
1:D:144:MET:HB3	1:D:144:MET:HE2	1.83	0.45
1:D:172:ASP:HA	1:D:176:ARG:NH2	2.32	0.45
1:D:125:GLU:O	1:D:129:ARG:HD2	2.16	0.45
1:D:126:GLU:CB	1:D:131:GLU:HG3	2.48	0.44
1:D:111:ARG:HA	1:D:111:ARG:HD3	1.75	0.44
1:D:207:ILE:HD11	1:D:212:ILE:CD1	2.39	0.44
1:D:129:ARG:HG3	1:D:181:VAL:CG1	2.46	0.44
1:A:161:LYS:O	1:A:239:ASP:HA	2.17	0.44
1:C:240:GLU:C	1:C:241:ILE:HD12	2.37	0.44
1:D:184:ASP:HB3	1:D:187:LYS:HB2	2.00	0.44
1:B:28:LYS:HE3	1:B:28:LYS:HB3	1.79	0.44
1:C:69:ILE:HB	1:C:73:GLU:CD	2.38	0.44
1:D:174:LYS:HE2	1:D:174:LYS:HB3	1.83	0.44
1:A:160:ILE:HA	1:A:240:GLU:O	2.18	0.44
1:B:110:LYS:HG2	1:B:248:THR:HG22	1.99	0.44
1:B:211:LYS:HA	1:B:211:LYS:HE2	2.00	0.44
1:A:160:ILE:HB	1:A:230:THR:HG22	1.99	0.43
1:D:290:MET:HG3	1:D:293:ILE:HD12	1.99	0.43
1:C:241:ILE:HD12	1:C:241:ILE:N	2.34	0.43
1:D:159:GLN:HA	1:D:229:SER:O	2.18	0.43
1:B:1:MET:CE	1:B:251:ALA:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HA	1:D:237:LEU:HD23	1.62	0.43
1:B:119:THR:HB	1:B:135:GLU:HG3	2.00	0.43
1:B:145:LYS:N	1:B:145:LYS:HD2	2.34	0.43
1:C:150:ASP:OD1	1:C:150:ASP:N	2.51	0.43
1:C:40:LYS:HB3	1:C:40:LYS:HE3	1.78	0.42
1:C:118:PHE:CD1	1:C:240:GLU:HG2	2.55	0.42
1:D:73:GLU:HA	1:D:73:GLU:OE1	2.19	0.42
1:A:311:ARG:HG3	1:C:342:PRO:HD2	2.02	0.42
1:A:86:THR:HA	1:A:90:MET:HE2	2.02	0.42
1:C:7:PHE:HZ	1:C:28:LYS:HE3	1.85	0.42
1:B:145:LYS:HA	1:B:145:LYS:CE	2.50	0.41
1:B:38:LEU:HD13	1:B:159:GLN:HG2	2.01	0.41
1:A:61[A]:MET:SD	1:B:61[A]:MET:HE3	2.61	0.41
1:B:1:MET:HE3	1:B:251:ALA:N	2.35	0.41
1:D:353:GLN:O	1:D:359:GLY:HA2	2.21	0.41
1:A:1:MET:HB2	1:A:102:VAL:O	2.21	0.41
1:A:119:THR:HB	1:A:135:GLU:CG	2.51	0.40
1:C:9:ILE:HD11	1:C:23:LEU:HD12	2.02	0.40
1:D:126:GLU:HB3	1:D:131:GLU:HG3	2.03	0.40
1:D:100:LYS:HE3	1:D:102:VAL:CG1	2.51	0.40
1:B:91:THR:OG1	1:D:311:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/363 (100%)	348 (96%)	14 (4%)	0	100	100
1	B	366/363 (101%)	353 (96%)	13 (4%)	0	100	100
1	C	360/363 (99%)	347 (96%)	13 (4%)	0	100	100
1	D	360/363 (99%)	346 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1448/1452 (100%)	1394 (96%)	54 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/286 (100%)	284 (99%)	3 (1%)	76 85
1	B	291/286 (102%)	285 (98%)	6 (2%)	53 64
1	C	285/286 (100%)	282 (99%)	3 (1%)	73 83
1	D	285/286 (100%)	276 (97%)	9 (3%)	39 47
All	All	1148/1144 (100%)	1127 (98%)	21 (2%)	59 70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ARG
1	A	239	ASP
1	A	282	ASP
1	B	73	GLU
1	B	145	LYS
1	B	236[A]	LEU
1	B	236[B]	LEU
1	B	239	ASP
1	B	290	MET
1	C	76	LYS
1	C	145	LYS
1	C	239	ASP
1	D	131	GLU
1	D	141	LYS
1	D	150	ASP
1	D	174	LYS
1	D	176	ARG

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Mol	Chain	Res	Type
1	D	210	ASP
1	D	237	LEU
1	D	239	ASP
1	D	283	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	249	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BR8	B	401	-	9,9,9	3.63	7 (77%)	12,12,12	3.93	7 (58%)
2	BR8	A	401[A]	-	9,9,9	4.11	7 (77%)	12,12,12	3.88	7 (58%)
2	BR8	C	401	-	9,9,9	3.55	5 (55%)	12,12,12	3.21	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BR8	D	401	-	9,9,9	3.60	6 (66%)	12,12,12	3.59	6 (50%)
3	MLI	A	402[B]	-	6,6,6	1.32	0	7,7,7	1.56	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	A	402[B]	-	-	2/4/4/4	-
2	BR8	B	401	-	-	-	0/1/1/1
2	BR8	A	401[A]	-	-	-	0/1/1/1
2	BR8	D	401	-	-	-	0/1/1/1
2	BR8	C	401	-	-	-	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	BR8	C2-N1	7.00	1.49	1.37
2	A	401[A]	BR8	C2-N3	6.31	1.48	1.37
2	B	401	BR8	C2-N3	6.14	1.48	1.37
2	C	401	BR8	C2-N1	6.02	1.47	1.37
2	D	401	BR8	C2-N3	5.96	1.47	1.37
2	C	401	BR8	C2-N3	5.81	1.47	1.37
2	D	401	BR8	C2-N1	5.77	1.47	1.37
2	B	401	BR8	C2-N1	5.45	1.46	1.37
2	A	401[A]	BR8	C4-N3	4.84	1.45	1.37
2	A	401[A]	BR8	C6-N1	4.84	1.45	1.37
2	B	401	BR8	C4-N3	4.49	1.45	1.37
2	D	401	BR8	C6-N1	4.46	1.45	1.37
2	C	401	BR8	C6-N1	3.97	1.44	1.37
2	D	401	BR8	C4-N3	3.75	1.44	1.37
2	C	401	BR8	C4-N3	3.64	1.43	1.37
2	B	401	BR8	C6-N1	3.63	1.43	1.37
2	C	401	BR8	O4-C4	-2.56	1.18	1.23
2	B	401	BR8	O4-C4	-2.49	1.18	1.23
2	A	401[A]	BR8	O8-C6	-2.26	1.18	1.23
2	B	401	BR8	O8-C6	-2.20	1.18	1.23
2	A	401[A]	BR8	O4-C4	-2.14	1.18	1.23
2	D	401	BR8	O2-C2	-2.05	1.19	1.23
2	B	401	BR8	O2-C2	-2.03	1.19	1.23
2	D	401	BR8	O4-C4	-2.01	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	BR8	O2-C2	-2.01	1.19	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401[A]	BR8	C4-N3-C2	-8.13	119.20	125.73
2	B	401	BR8	C6-N1-C2	-8.01	119.29	125.73
2	D	401	BR8	C6-N1-C2	-7.98	119.32	125.73
2	A	401[A]	BR8	C6-N1-C2	-7.62	119.60	125.73
2	B	401	BR8	C4-N3-C2	-7.44	119.75	125.73
2	C	401	BR8	C4-N3-C2	-7.24	119.91	125.73
2	D	401	BR8	C4-N3-C2	-6.92	120.16	125.73
2	B	401	BR8	C5-C6-N1	5.78	122.32	116.82
2	C	401	BR8	C6-N1-C2	-5.76	121.10	125.73
2	A	401[A]	BR8	C5-C6-N1	4.55	121.15	116.82
2	D	401	BR8	C5-C6-N1	4.27	120.88	116.82
2	A	401[A]	BR8	C5-C4-N3	3.53	120.18	116.82
2	C	401	BR8	C5-C4-N3	3.51	120.16	116.82
2	C	401	BR8	C5-C6-N1	3.36	120.02	116.82
2	B	401	BR8	O8-C6-C5	-3.17	117.69	122.85
2	B	401	BR8	C5-C4-N3	3.05	119.72	116.82
2	A	401[A]	BR8	O8-C6-C5	-2.83	118.24	122.85
3	A	402[B]	MLI	O9-C3-C1	2.65	122.99	114.54
2	D	401	BR8	N3-C2-N1	2.61	119.99	115.80
2	A	401[A]	BR8	N3-C2-N1	2.53	119.88	115.80
3	A	402[B]	MLI	O8-C3-C1	-2.38	115.12	122.08
2	D	401	BR8	O8-C6-C5	-2.35	119.02	122.85
2	D	401	BR8	C5-C4-N3	2.32	119.03	116.82
2	B	401	BR8	N3-C2-N1	2.26	119.44	115.80
2	B	401	BR8	O4-C4-C5	-2.25	119.19	122.85
2	A	401[A]	BR8	O2-C2-N3	-2.03	117.98	121.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402[B]	MLI	C3-C1-C2-O7
3	A	402[B]	MLI	C3-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	BR8	1	0
2	A	401[A]	BR8	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	362/363 (99%)	-0.24	4 (1%) 80 80	26, 40, 70, 142	0
1	B	363/363 (100%)	-0.33	0 100 100	27, 42, 68, 92	0
1	C	362/363 (99%)	-0.23	2 (0%) 89 89	29, 50, 81, 151	0
1	D	362/363 (99%)	0.49	36 (9%) 7 7	33, 74, 129, 164	0
All	All	1449/1452 (99%)	-0.08	42 (2%) 51 52	26, 47, 98, 164	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	LYS	7.9
1	D	177	GLY	7.4
1	D	242	ILE	5.6
1	D	106	ALA	5.6
1	A	107	ALA	5.1
1	D	107	ALA	4.8
1	D	140	VAL	4.8
1	D	108	PRO	4.7
1	D	207	ILE	4.6
1	D	109	GLY	4.6
1	D	136	VAL	4.5
1	D	103	ALA	4.4
1	D	170	ILE	4.2
1	C	107	ALA	4.2
1	D	280	ARG	4.1
1	D	367	VAL	4.0
1	D	105	PRO	4.0
1	D	122	PHE	3.9
1	D	212	ILE	3.9
1	A	106	ALA	3.9
1	D	150	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	175	ARG	3.6
1	D	114	VAL	3.4
1	A	108	PRO	3.4
1	D	236	LEU	3.4
1	D	168	GLU	2.8
1	D	203	ALA	2.5
1	A	280	ARG	2.5
1	D	251	ALA	2.4
1	D	366	ARG	2.4
1	D	69	ILE	2.4
1	D	102	VAL	2.3
1	D	176	ARG	2.3
1	C	106	ALA	2.3
1	D	63	LEU	2.2
1	D	97	PHE	2.2
1	D	128	GLY	2.2
1	D	149	ILE	2.1
1	D	116	VAL	2.1
1	D	104	ALA	2.1
1	D	74	VAL	2.0
1	D	217	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BR8	A	401[A]	9/9	0.95	0.10	32,35,42,42	13
2	BR8	B	401	9/9	0.97	0.10	29,31,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BR8	C	401	9/9	0.97	0.10	32,35,41,43	0
4	CA	D	402	1/1	0.97	0.05	66,66,66,66	0
3	MLI	A	402[B]	7/7	0.98	0.10	30,35,42,42	9
2	BR8	D	401	9/9	0.98	0.09	42,45,53,55	0
4	CA	C	402	1/1	0.99	0.07	37,37,37,37	1
4	CA	A	403	1/1	1.00	0.12	37,37,37,37	1
4	CA	B	402	1/1	1.00	0.07	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.